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Brownian dynamics approach to interacting magnetic moments

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The question how to introduce thermal fluctuations in the equation of motion of a magnetic system is addressed. Using the approach of the fluctuation-dissipation theorem we calculate the properties of the noise for both, the fluctuating field and fluctuating torque (force) representation. In contrast to earlier calculations we consider the general case of a system of interacting magnetic moments without the assumption of axial symmetry. We show that the interactions do not result in any correlations of thermal fluctuations in the field representation and that the same widely used formula can be used in the most general case. We further prove that close to the equilibrium where the fluctuation-dissipation theorem is valid, both, field and torque (force) representations coincide, being different far away from it.

The problem of a correct introduction of temperature in the equation of motion of a magnetic system has gained much importance as a result of technological requirements of magnetic recording industry [1, 2, 3]. This is associated with the need to perform calculations of magnetization dynamics at finite temperatures. Open problems include fast magnetization switching, thermal stability and magnetic viscosity, among others. The correct solution of the problem is still far from being understood. The main difference between the magnetic problem and the standard molecular dynamics approach is that the magnetic moment dynamics is governed by the Landau-Lifshitz equation which includes the precession of a magnetic moment around its internal field direction. It comprises coupled first-order equations for the magnetization components, and the requirement of conservation of the magnetization amplitude. As a consequence, no analogue of mass and kinetic energy exist in the system, thus making it impossible to introduce the temperature through this mechanism.

Consequently, the temperature is introduced through small deviations from the equilibrium configuration. Therefore, strictly speaking, this approach is only valid when these deviations are small and it cannot be used for fast magnetization switching.

Let us briefly summarize the original approach from W. Brown [4, 5]. The underlying equation of motion is the Landau-Lifshitz-Gilbert equation which can be written in the form

$$\frac{d\overrightarrow{\mathbf{M}}_i}{d\tau} = -\overrightarrow{\mathbf{M}}_i \times \overrightarrow{\mathbf{H}}_i - \alpha \overrightarrow{\mathbf{M}}_i \times [\overrightarrow{\mathbf{M}}_i \times \overrightarrow{\mathbf{H}}_i], \qquad (1)$$

where

$$\tau = \frac{\gamma_0 H_k}{M_s(1+\alpha^2)} t, \quad \overrightarrow{\mathbf{H}} = -\frac{\delta E^*}{\delta \overrightarrow{\mathbf{M}}} \qquad (2)$$

γ_0 is the gyromagnetic ratio and α is the damping constant. The magnetic moment $\overrightarrow{\mathbf{M}}$ is normalized to the saturation value M_s, and the internal field $\overrightarrow{\mathbf{H}}$ is normalized to the anisotropy field $H_k = 2K/M_s$. The energy $E^* = E/2KV$, where K is the anisotropy value and V is the particle volume, contains all the necessary energy contributions: anisotropy, exchange, magnetostatic and Zeeman.

W. Brown proposed the inclusion of thermal fluctuations via a random field, added to the internal field, Eq. 2. For the calculation of the properties of the random field he outlined two methods: (i) based on the fluctuation-dissipation theorem (see also [6]) and (ii) by imposing the condition that the equilibrium solution of the correspondent Fokker-Planck equation is the Boltzmann distribution (see also [7]). As a result of both the thermal field statistical properties are given by

$$\langle \xi_i \rangle = 0, \quad \langle \xi_i(0)\xi_j(\tau) \rangle = \frac{\alpha k_B T}{KV(1+\alpha^2)} \delta_{ij}\delta(\tau), \qquad (3)$$

where i, j denote Cartesian components x, y, z. Different approaches based, for example, on the Landau-Lifshitz rather than on the Landau-Lifshitz-Gilbert equation were also introduced [7, 8].

However, the properties of the thermal noise, Eqs. 3, were derived only for one isolated particle. Moreover, Brown considered in his paper [4] only the simplest axially symmetric case. Nevertheless, in the past the formulas above provided the basis for practically every numerical method [2, 9, 10, 11] for the computation of magnetization dynamics taking into account thermal fluctuations. But the investigated magnetic systems usually comprise interacting particles [12, 13, 14, 15, 16, 17] due to magnetostatic and/or exchange couplings. For that

case the thermal field may be expected to be influenced by correlations between different particles [10]. Hence, it is necessary to generalize Brown's result to the case of interacting magnetic moments. To the best of our knowledge, this has never been done before.

In what follows we start with the Brownian dynamics approach (see [18]) which was originally applied to magnetic systems by A. Lyberatos et al. [6, 10]. However, we consider the general case of an interacting system with a non-axially-symmetric potential. Following the standard approach, we introduce the temperature into the motion of the Brownian particles (i. e. the magnetic moments) as a result of the fluctuation-dissipation theorem. Consequently, this approach is only valid when small deviations from equilibrium are considered.

The general Langevin equation of motion is written in the form

$$\frac{dx_i}{dt} = -\sum_j \gamma_{ij} X_j + f_i, \quad X_j = -\frac{\partial S}{\partial x_j}, \tag{4}$$

where the γ_{ij} are the so-called kinetic coefficients, X_j are variables which are thermodynamically conjugate to x_j, and S is the entropy of the magnetic system. For a closed system in an external medium,

$$X_j = \frac{1}{k_B T}\frac{\partial E}{\partial x_j}. \tag{5}$$

In Eq. 4, f_i is a random force representing thermal fluctuations in the system having the properties

$$\langle f_i(t)\rangle = 0 \quad \text{and} \quad \langle f_i(0) f_j(t)\rangle = \mu_{ij}\delta(t) \tag{6}$$

where

$$\mu_{ij} = \gamma_{ij} + \gamma_{ji}. \tag{7}$$

A linear equation of motion of the form

$$\frac{dx_i}{dt} = \sum_j L_{ij} x_j, \tag{8}$$

with the associated energy

$$E = E_0 + \frac{1}{2}\sum_{i,j} A_{ij} x_i x_j, \tag{9}$$

can be rewritten as

$$\frac{dx_i}{dt} = -\sum_j L_{ij} x_j = -\sum_j \gamma_{ij} \frac{1}{k_B T}\sum_k A_{kj} x_k, \tag{10}$$

so that the matrix L_{ik} is related to the kinetic coefficients γ_{ik} in the following way [6]:

$$L_{ik} = -\frac{1}{k_B T}\sum_j \gamma_{ij} A_{kj} \tag{11}$$

In micromagnetics the motion of a magnetic moment $\mathbf{M}$ is governed by the deterministic LLG equation (Eq. 1). For the equilibrium state of the system Brown's condition

$$\overrightarrow{\mathbf{M}_i^0} \times \overrightarrow{\mathbf{H}_i^0} = 0 \tag{12}$$

must be satisfied, implying that here $\overrightarrow{\mathbf{H}_i^0}$ and $\overrightarrow{\mathbf{M}_i^0}$ are parallel. Close to equilibrium, the LLG equation can be linearized using small deviations

$$\overrightarrow{\mathbf{m}_i} = \overrightarrow{\mathbf{M}_i} - \overrightarrow{\mathbf{M}_i^0}, \quad \overrightarrow{\mathbf{h}_i} = \overrightarrow{\mathbf{H}_i} - \overrightarrow{\mathbf{H}_i^0} \tag{13}$$

from their equilibrium values, yielding

$$\frac{dm_i}{dt} = \sum_{j=1}^{3N} L_{ij} m_j. \tag{14}$$

Here, the indices i, j count the particles sites $1, ..., N$ as well as their x, y, z coordinates. The internal fields h_j play the role of the variables which are thermodynamically conjugate to m_j,

$$X_j = \frac{1}{k_B T}\frac{\partial E}{\partial m_j} = -\frac{2KV}{k_B T} h_j. \tag{15}$$

Thus, the LLG equation should be rewritten in the form

$$\frac{dm_i}{dt} = \frac{2KV}{k_B T}\sum_{j=1}^{3N} \gamma_{ij} h_j \tag{16}$$

which is an easier way to calculate the kinetic coefficients than the use of Eq. 11. The representation of the LLG equation in the form of Eq. 4 means that in what follows the thermal fluctuations are introduced as a fluctuating torque (a generalized force rather than a field). Later we will show that in the linear approximation this is equivalent to the standard fluctuating field representation. Alternatively, Eq. 16 could be viewed as a polar representation of the magnetization vector $m_i^1 = \theta_i, m_i^2 = \varphi_i$, in this case the conjugate variables are the polar projections of the internal fields (h_θ, h_φ) and the fluctuations f_i will stand for the random field polar components. This latter approach was used originally by W. Brown [4].

We continue by writing the energy of the system in the form

$$E^* = \sum_i^N \big(-\overrightarrow{\mathbf{M}_i}\cdot\overrightarrow{\mathbf{H}_i} + \frac{\lambda}{2}\mathbf{M}_i^2\big). \tag{17}$$

where λ is the Lagrange multiplier. In the zero order approximation one obtains

$$\overrightarrow{\mathbf{M}_i^0} = \frac{1}{\lambda}\overrightarrow{\mathbf{H}_i^0} \tag{18}$$

which corresponds to Brown's condition, Eq. 12. The linear approximation leads to the equilibrium condition

$$-\overrightarrow{\mathbf{M}_i^0}\cdot\overrightarrow{\mathbf{h}_i} - \overrightarrow{\mathbf{H}_i^0}\cdot\overrightarrow{\mathbf{m}_i} + \lambda\overrightarrow{\mathbf{M}_i^0}\cdot\overrightarrow{\mathbf{m}_i} = 0, \tag{19}$$

which leaves us only the quadratic form for the energy expression near the equilibrium,

$$E^* = E_0 - \sum_i^N \left(\overrightarrow{\mathbf{m}_i} \cdot \overrightarrow{\mathbf{h}}_i - \frac{\lambda}{2}\mathbf{m}_i^2\right). \qquad (20)$$

The general expression for magnetic energies is a quadratic form in terms of the magnetization (apart from the Zeeman term which is included in the equilibrium field $\overrightarrow{\mathbf{H}_i^0}$ and condition 19). Therefore, it is reasonable to suppose that the total field can be expressed as

$$h_i^\alpha = \sum_{j,\beta} B_{ij}^{\alpha\beta} m_j^\beta = h_{eff,i}^\alpha - \lambda m_i^\alpha \qquad (21)$$

where $h_{eff,i}^\alpha$ are the components of the effective field due to the different energy contributions and $-\lambda m_i^\alpha$ is the field due to the kinematic interaction expressing the constraints (Lagrange multiplier). The value of the Lagrange multiplier is normally found from the equilibrium condition 19. However, its actual value is not necessary for calculations due to the fact that the LLG equation conserves the magnetization length. Latin indices represent the sites of the moments and the Greek ones the magnetization components x, y, z. In this case the final expression for the energy (Eq. 20) takes the form

$$E^* = E_0 - \sum_{i,j,\alpha,\beta} (B_{ij}^{\alpha\beta} - \delta_{ij}\delta_{\alpha\beta}) m_i^\alpha m_j^\beta. \qquad (22)$$

The expressions for the kinetic coefficients could be obtained by using directly the expression 11. In this approach it seems that the final result could also include correlations between different particles [10]. But this is not the case: the kinetic coefficients can be obtained much easier representing the linearized LLG equation in the form of Eq. 16 yielding

$$\begin{aligned}
\gamma_{ij}^{xx} &= \frac{\alpha k_B T}{2KV}\left[(M_i^{0,y})^2 + (M_i^{0,z})^2\right]\delta_{ij} && (23)\\
\gamma_{ij}^{xy} &= \frac{k_B T}{2KV}\left[-M_i^{0,z} + \alpha M_i^{0,x} M_i^{0,y}\right]\delta_{ij} && (24)\\
\gamma_{ij}^{yx} &= \frac{k_B T}{2KV}\left[M_i^{0,z} + \alpha M_i^{0,x} M_i^{0,y}\right]\delta_{ij} && (25)\\
\gamma_{ij}^{yy} &= \frac{\alpha k_B T}{2KV}\left[(M_i^{0,x})^2 + (M_i^{0,z})^2\right]\delta_{ij}. && (26)
\end{aligned}$$

The other coefficients can be obtained by symmetry. Note, that there are no correlations between different particles. Also, the kinetic coefficients have obviously reversible parts (coming from rotation) and irreversible parts (from damping). The reversible antisymmetric parts do not contribute to the thermal fluctuations after adding the kinetic coefficients to calculate the matrix μ from Eq. 7, yielding

$$\begin{aligned}
\mu_{ij}^{xx} &= \frac{\alpha k_B T}{KV}\left[(M_i^{0,y})^2 + (M_i^{0,z})^2\right]\delta_{ij} && (27)\\
\mu_{ij}^{xy} &= \frac{\alpha k_B T}{KV} M_i^{0,x} M_i^{0,y}\delta_{ij}. && (28)
\end{aligned}$$

Once again, the others can be obtained by symmetry. Note that in a general system of coordinates there are correlations between different magnetization components but no correlations between different particles. However, if we set the local coordinate system such that the z axis coincides with the equilibrium magnetization direction, $M_i^{0,x} = 0, M_i^{0,y} = 0, M_i^{0,z} = 1$, these correlations disappear and we have the same thermal fluctuations in x and y directions but no fluctuations in z direction,

$$\mu_{ij}^{xx} = \mu_{ij}^{yy} = \frac{\alpha k_B T}{KV}\delta_{ij} \quad \text{and} \quad \mu_{ij}^{zz} = 0. \qquad (29)$$

Thus, the torque fluctuations produce effectively correlations and different values of thermal fluctuations in all other systems of coordinates different from the global one, where one of the axes is parallel to the equilibrium magnetization direction and where the equation of motion for this component disappears.

It is customary to introduce thermal fluctuations in the field components (see [9] and originally W. F. Brown [4]) instead of the torque fluctuations as derived above. This has its origin in the representation of the LLG equation in a spherical system of coordinates in form of Eq. 4. However, in both of these papers above only the axially symmetric case without interactions was considered. The big difference between these two approaches is the *multiplicative* character of the field noise versus the *additive* noise of the torque. This turns out to be important for larger magnetization deviations. But first we will show that in the global coordinate system both approaches, torque and field, give the same result, as long as the magnetization deviations from the equilibrium are small.

Let us use a decomposition of the field components according to $H^i \to H^i + \xi^i$, where ξ^i are the components of the fluctuation part of the field. When this is done we obtain the following expansion of the equations of motion,

$$\begin{aligned}
\frac{dM^i}{d\tau} &= -\varepsilon^{ijk} M^j H^k - \alpha H^m \left[M^m M^i - \delta^{mi}\right]\\
&\quad -\varepsilon^{ijk} M^j \xi^k - \alpha \xi^m \left[M^m M^i - \delta^{mi}\right]\\
&= A^i(M^n, H^l) + B^{ij}(M^n)\xi^j. && (30)
\end{aligned}$$

Furthermore, in the global system of coordinates we linearize the magnetization by the decomposition $M^i \to M_0^i + m^i$, where m^i are $s$mall fluctuations around the equilibrium values M_0^i, and apply the constraint condition, $|\overrightarrow{\mathbf{M}}| = 1$. For simplicity below we drop in the formulas the particle index i. The components in the specified coordinate system are then

$$\begin{aligned}
\frac{dm^x}{d\tau} &= A^x(\overrightarrow{m}) - (m^y + \alpha m^x)\,\xi^z + f^x, && (31)\\
\frac{dm^y}{d\tau} &= A^y(\overrightarrow{m}) + (m^x - \alpha m^y)\,\xi^z + f^y, && (32)\\
\frac{dm^z}{d\tau} &= (m^x + m^y)\,(\xi^x - \alpha\xi^y)\,, && (33)
\end{aligned}$$

where $\overrightarrow{A}(\overrightarrow{m})$ stands for the linearized deterministic part of the LLG equation and

$$f^x = \xi^y + \alpha\xi^x, \quad f^y = -\xi^y + \alpha\xi^x. \tag{34}$$

The constraint condition implies that in a first order approximation it is $m^z(\tau) = 0, \ \forall\tau$. This is compatible with Eq. 33 only if the field fluctuations ξ^i can be considered to be small quantities, in which case products of the ξ^i with the m^i can be ignored in Eq.(31). These equations suggest that the field fluctuations contribute *additively.* From Eqs. 34 one can also obtain Brown's formulas for the field fluctuations (Eq. 3).

It is important to note that the last equation is satisfied for any fluctuation field value due to the character of the LLG equation. Thus the f^z value (or ξ^z) is in this case undefined. In any case the component ξ^z is not efficient since it acts parallel to the magnetization direction. The assumption made in the paper of A. Lyberatos and R. Chantrell [9] is that the field components are isotropic and that

$$\langle\xi^x\rangle = \langle\xi^y\rangle = \langle\xi^z\rangle. \tag{35}$$

This assumption in the global system of coordinates (where the fluctuation-dissipation theorem is applied) leads to the remarkable symmetry (35) of the field components in all the systems of coordinates and to the absence of correlations. Furthermore, it is assumed that this property is valid through the magnetization reversal.

For the torque fluctuations the reasonable hypothesis to mimic the field ones would be the assumption that there are never torque (force) fluctuations along the magnetization direction. In this case the correlations between different noise components would appear in all other systems of coordinates different from the global one. While equivalent near the equilibrium, these two approaches will be different far from it. At this point, we would like to restate that the whole theory is valid for small fluctuations around the equilibrium where both approaches coincide.

In conclusion, the application of the Brownian dynamics approach to the motion of a magnetic system shows that interactions do not introduce correlations into thermal fluctuations introduced as both, either a fluctuating torque or a fluctuating field. Correlations may appear between different magnetization components as a result of the conservation of the value of the magnetic moment. The reasonable hypothesis that all the fluctuating field components are equivalent leads to Brown's well-known formulas for the fluctuating fields values without correlations. This validates all previously done micromagnetic calculations where this kind of assumption was made.

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